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EFFECTS OF HETEROGENEOUS AND HOMOGENEOUS REACTIONS ON THE DISPERSION OF A SOLUTE IN SIMPLE MICROFLUID

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In this paper the dispersion of a solute matter in a simple microfluid flow through a channel has been discussed. The effects of homogeneous and heterogeneous reaction rates have been considered in the analysis using Taylor's limiting condition and the effects of various parameters on the equivalent dispersion coefficient have been studied. It is observed that for a given simple microfluid the combined effect of homogeneous and heterogeneous chemical reaction is to decrease the equivalent dispersion coefficient.

1. INTRODUCTION

The dispersion of a solute in fluid flowing through channels/pipes is important in chemical as well as biological systems. In one of the early studies, Taylor[10] presented a simple mathematical model to study dispersion of a solute through a fluid. He observed that, relative to a plane moving with the average speed of the flow, the solute disperses with an equivalent dispersion coefficient which depends upon (i) the average speed of the flow, (ii) the radius of the tube, and (iii) the molecular diffusion coefficient. In his analysis, Taylor[10] assumed that the solute does not chemically react with the fluid. However, in a variety of problems in chemical engineering, diffusion of solute takes place in the presence of irreversible first order chemical reaction. Therefore, many investigators analyed the dispersion problem by considering first order homogeneous reaction, under laminar flow conditions. Further, the wall of the channel may be catalytic, which in turn gives rise to heterogeneous chemical reaction at the surface. Katz[5] discussed the influence of the heterogeneous chemical reaction catalyzed on the wall of the tube. The combined effects of homogeneous and heterogeneous chemical reaction for a solute dispersing in Newtonian fluid flow have been discussed by Walker[11], Solomon and Hudson[7], Gupta and Gupta[3] and others.

It may be noted that many of the fluids are suspensions of particulate matter in microscopically continuous fluids. Eringen[2] introduced the concept of simple microfluids to characterize concentrated suspensions of neutrally buoyant deformable particles in a viscous fluid. Such fluid model can be used to rheologically describe polymer suspensions, normal human blood etc. In the above mentioned investigations such characterization has not been considered. For a sub class of these microfluids, known as micropolar fluids, Soundalgekar[8] studied the dispersion of a solute in the laminar flow of a micropolar fluid in a channel. In a subsequent paper Soundalgekar and Chaturani[9] considered the effect of couple stress on the dispersion of a solute matter in a pipe flow. Chandra and Agarwal[1] considered dispersion of solute in a simple microfluid flow when the first order irreversible chemical reaction in fluid is taking place. However, they did not consider the effect of chemical reaction catalyzed at the wall. Hence, in this paper we study the combined effects of homogeneous and heterogeneous chemical reaction of a solute in a suspension of neutrally buoyant particles, which is modelled as a simple microfluid, flowing through a channel.

2. Mathematical Formulation

We consider here dispersion of a solute in a steady flow of a simple microfluid, between two parallel plates (distance $2h$ apart). The flow is assumed to be laminar and one-dimensional under a uniform pressure gradient $\frac{dp}{dz} = P$ (The co-ordinate system o-xyz is such that, z-axis lies along the length of the channel and is shown in Fig. 1). Further we assume that the solute, which is present in small concentration, diffuses and simultaneously undergoes a first order irreversible chemical reaction in the fluid under isothermal condition. Thus, the equation for concentration, c is given by, Gupta and Gupta[3], Shukla *et al.*[6]

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial z} = D\frac{\partial^2 c}{\partial x^2} - Kc. \qquad \text{... (1)}$$

Here the equation is written by neglecting the axial diffusion and the term $-Kc$ represents volume rate of disappearance of the solute, D, is constant molecular diffusion coefficient, K is the first order homogeneous chemical reaction rate constant and v is the velocity of the simple microfluid along the z-axis.

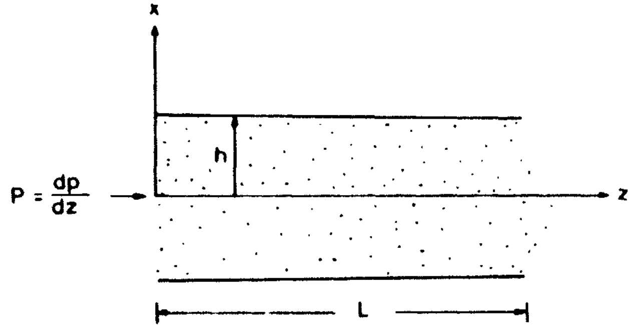

Fig. 1. Geometry of the problem

Further, assuming that the walls of the channel are catalytic (hence, allow a heterogeneous chemical reaction) the differential material balance at the walls gives, Katz[5], Gupta and Gupta[3].

$$\left.\begin{aligned} -D\frac{\partial c}{\partial x} &= fc \qquad \text{at } x = h \\ -D\frac{\partial c}{\partial x} &= -fc \qquad \text{at } x = -h \end{aligned}\right\} \qquad \dots (2)$$

where, fc gives the surface reaction rate.

Following Taylor[10] eqn. (1) can be written relative to the axis moving with mean fluid velocity ($\bar{v}$) which on using the dimensionless variables.

$$\bar{z} = \frac{z - \bar{v}t}{h}, \qquad \bar{x} = \frac{x}{h} \qquad \dots (3)$$

becomes,

$$\frac{\partial c}{\partial t} + \frac{v - \bar{v}}{h}\frac{\partial c}{\partial \bar{z}} = D\frac{\partial^2 c}{\partial \bar{x}^2} - Kc \qquad \dots (4)$$

$\bar{v}$ is average fluid velocity given by,

$$\bar{v} = \frac{1}{h}\int_0^h v\, dx. \qquad \dots (5)$$

Assuming that the Taylor's limiting condition is valid i.e. the partial equilibrium is established in any cross-section of the channel, eqn. (4) reduces to

$$\frac{\partial^2 c}{\partial \bar{x}^2} - m^2 c = \frac{h}{D}\frac{\partial c}{\partial \bar{z}}(v - \bar{v}) \qquad \dots (6)$$

where $\frac{\partial c}{\partial \bar{z}}$ is independent of $\bar{x}$, $\frac{\partial c}{\partial t} = 0$ and $m^2 = \frac{Kh^2}{D}$ characterizes the chemical reaction rate.

The boundary condition (2) can be rewritten as

$$\left.\begin{aligned} \frac{\partial c}{\partial \bar{x}} + \gamma c &= 0 \qquad \text{at } \bar{x} = 1 \\ \frac{\partial c}{\partial \bar{x}} - \gamma c &= 0 \qquad \text{at } \bar{x} = -1 \end{aligned}\right\} \qquad \dots (7)$$

where $\gamma = \frac{hf}{D}$ is the surface reaction rate constant.

Now to solve the equation (6) for concentration c, we need the expression of velocity $\vec{v}$ of the simple microfluid. As, the flow is laminar and one dimensional we take $\vec{v} = (0, 0, v(z))$ and the non-zero components of the gyration tensor ν_{kl} as $\nu_{13}(z)$ and $\nu_{31}(z)$ only, Kang and Eringen[4]. It may be pointed out here that the symmetric and skew symmetric parts of the gyration tensor ν_{kl} characterize the deformation and rotation of suspended particles respectively. Thus, the governing equations for the flow of simple microfluid in a channel can be written as, Chandra and Agarwal[1].

$$\frac{1}{h} v'' - E_1 \nu'_{(13)} + E_3 \left(\frac{v'}{2h} + \nu'_{[13]} \right) - hP = 0 \qquad \dots (8)$$

$$(\overline{K}_1 + \overline{K}_3) \nu''_{31} + (\overline{K}_2 + \overline{K}_4) \nu''_{13} - 2(E_1 + 2E_2) \nu_{(13)}$$

$$- E_3 \left(\frac{v'}{h} + 2 \nu_{[13]} \right) = 0 \qquad \dots (9)$$

$$(\overline{K}_1 - \overline{K}_3) \nu''_{31} + (\overline{K}_2 - \overline{K}_4) \nu''_{13} - 2(E_1 + 2E_2) \nu_{(13)}$$

$$+ E_3 \left(\frac{v'}{h} + 2 \nu_{[13]} \right) = 0. \qquad \dots (10)$$

Here $\nu_{(13)}$, $\nu_{[13]}$ are the symmetric and skew-symmetric parts of ν_{13} respectively, $(\ )' = \frac{d}{d\overline{x}} (\ )$; E_1, E_2, E_3 are dimensionless viscosity coefficients and K_i are nondimensional simle micro fluid parameters (Chandra and Agarwal[1]).

The boundary conditions for v, ν_{13}, ν_{31} are taken as follows, Kang and Eringen[4], Chandra and Agarwal[1]

$$\left.\begin{array}{l} \text{(i)} \quad v = 0 \,;\ \nu_{(13)} = \dfrac{A_1}{h} v' \,;\ \nu_{[13]} = \dfrac{A_2}{h} v' \ \text{ at } \overline{x} = 1 \\ \text{(ii)} \quad v' = 0 \,;\ \nu_{(13)} = 0 \quad ;\ \nu_{[13]} = 0 \ \text{ at } \overline{x} = 0 \end{array}\right\} \qquad \dots (11)$$

Solving the above equations (8) to (10) along with the boundary conditions (11) the expressions for $\nu_{(13)}$, $\nu_{[31]}$, v can be obtained as (Chandra and Agarwal[1]),

$$\nu_{(13)} = -\frac{Ph}{2\mu} \left[\frac{b_1}{2} (1 + f_1) \frac{\sinh \overline{\alpha} \overline{x}}{\sinh \overline{\alpha}} + \frac{b_2}{2} (1 + f_2) \frac{\sinh \overline{\beta} \overline{x}}{\sinh \overline{\beta}} \right] \qquad \dots (12)$$

$$\nu_{(13)} = -\frac{Ph}{2\mu} \left[\overline{x} + \frac{b_1}{2} (1 + f_1) \frac{\sinh \overline{\alpha} \overline{x}}{\sinh \overline{\alpha}} + \frac{b_2}{2} (1 - f_2) \frac{\sinh \overline{\beta} \overline{x}}{\sinh \overline{\beta}} \right] \qquad (13)$$

$$v = -\frac{Ph^2}{2\mu} [1 - \overline{x}^2 + d_1 (\cosh \overline{\alpha} - \cosh \overline{\alpha} \overline{x})$$

$$+ d_2 (\cosh \overline{\beta} - \cosh \overline{\beta} \overline{x})] \qquad \dots (14)$$

where,

$$b_1 = [-2A_1 h_2 + (1 + 2A_2) g_2] / [g_1 h_2 - g_2 h_1]$$

$$b_2 = [-2A_1 h_1 + (1+2A_2) g_1]/[g_1 h_2 - g_2 h_1]$$

$$d_i = -\frac{b_i e_i}{a_i \sinh a_i}$$

$$g_i = (-1)^{i+1}\left\{\frac{(1+f_i)}{2} - A_1 e_i\right\}$$

$$h_i = (-1)^{i+1}\left\{\frac{(1-f_i)}{2} - A_2 e_i\right\}$$

$$f_i = \frac{(a_i^2 - \overline{\alpha}_4^2)\overline{K}_1\overline{K}_4 + (a_i^2 - \overline{\alpha}_2^2)\overline{K}_2\overline{K}_3}{K_1 K_3 (\alpha_1^2 - \alpha_3^2)}$$

$$e_i = \frac{(E_1 - E_3) + (E_1 + E_3) f_i}{(2 + E_3)}$$

$$K_1\ \overline{\alpha}_1^2 = (E_1 + 2E_2) = \overline{K}_2 \overline{\alpha}_2^2$$

$$(2 - E_1)/\overline{K}_3\ \overline{\alpha}_3^2 = (1 + 2/E_3) = (2 + E_1)/K_4\ \alpha_4^2\ ,$$

$$a_1 = \overline{\alpha}\ ;\ a_2 = \overline{\beta},$$

are given as the roots of the equation :

$$(\overline{K}_1\ \overline{K}_4 + \overline{K}_2\ \overline{K}_3)\ x^2 + [\ (\overline{\alpha}_1^2 + \overline{\alpha}_4^2)\overline{K}_1\ \overline{K}_4 + (\overline{\alpha}_2^2 + \overline{\alpha}_3^2)\ \overline{K}_2\ \overline{K}_3\ ]$$

$$+ \overline{\alpha}_1^2\ \overline{\alpha}_4^2\ \overline{K}_1\ \overline{K}_4 + \overline{\alpha}_2^2\ \overline{\alpha}_3^2\ \overline{K}_2\ \overline{K}_3 = 0. \quad \dots (15)$$

Thus the average velocity of the fluid is obtained as

$$\overline{v} = -\frac{Ph^2}{2\mu}\left[\frac{2}{3} + d_1\left(\cosh\overline{\alpha} - \frac{\sinh\overline{\alpha}}{\overline{\alpha}}\right) + d_2\left(\cosh\overline{\beta} - \frac{\sinh\overline{\beta}}{\overline{\beta}}\right)\right] \quad \dots (16)$$

Solving equation (6) using the equations (14), (16) and the boundary conditions (7), we get

$$c = c^*\left\{\frac{2}{m^4} + \frac{\overline{x}^2}{m^2} - \frac{1}{m^2}\left[1 + \frac{6\cosh m\overline{x}}{F_4(\gamma\ ,\ m)}\right.\right.$$

$$\left.\left. - \sum_{i=1}^{2} d_i \left\{\frac{\sinh a_i}{a_i}\left(\frac{1}{m^2} - \frac{a_i^2 \cosh m\overline{x}}{m(a_i^2 - m^2)\sinh m}\right) + \frac{\cosh a_i \overline{x}}{a_i^2 - m^2}\right\}\right]\right\}$$

$$+ \frac{c^*\gamma}{F_4(\gamma\ ,\ m)}\left[\ 2\, m \cosh m\overline{x}\, F_1(m, \overline{\alpha}\ ,\ \beta) - 2\sinh m\, F_2(m, \overline{\alpha}, \beta)\right.$$

$$\left. + 2\gamma \sinh m\, F_1(m, \overline{\alpha}, \beta)\ \right] \quad \dots (17)$$

where, $c^* = \frac{h v_0}{D} \frac{\partial c}{\partial \bar{z}}, \quad v_0 = \frac{P h^2}{2\mu}$

$$F_1(m, \bar{\alpha}, \bar{\beta}) = \left[F_3(m, \bar{\alpha}, \beta) - \frac{1}{m^2} + \sum_i \frac{d_i}{a_i^2 - m^2} \cosh a_i \right]$$

$$F_2(m, \bar{\alpha}, \bar{\beta}) = \left[\frac{2}{m^2} - \sum_i \frac{d_i a_i}{a_i^2 - m^2} \sinh a_i \right]$$

$$F_3(m, \bar{\alpha}, \bar{\beta}) = \left[\frac{1}{m^2} \left(\frac{1}{3} - \frac{2}{m^2} + \sum_i \frac{d_i \sinh a_i}{a_i} \right) \right]$$

$$F_4(\gamma, m) = [\sinh m \{m^2 + \gamma^2\} + 2\gamma m \cosh m]$$

where, the summation index, i, takes the value 1 and 2.

The average solute flux, Q, across the plane which moves with the mean speed of the flow can be obtained from,

$$Q = 2h \int_0^1 c(\bar{x})(v - \bar{v})\, d\bar{x}. \qquad \text{... (18)}$$

Substituting the expression of v and $\bar{v}$ from eqn. (14) and eqn. (16) in eqn. (18) we get,

$$\frac{Q}{2h} = \left(-\frac{v_0^2 h}{2D} \frac{\partial c}{\partial \bar{z}} \right) M_1(m, \bar{\alpha}, \bar{\beta}, \gamma) \qquad \text{... (19)}$$

where,

$$M_1(m, \bar{\alpha}, \beta, \gamma) = \left[\frac{1}{3} + d_1 \frac{\sinh \bar{\alpha}}{\bar{\alpha}} + d_2 \frac{\sinh \bar{\beta}}{\bar{\beta}} \right]$$

$$\left[F_5 \frac{\sinh m}{m} - F_3(m, \bar{\alpha}, \beta) + \frac{1}{3m^3} - \frac{d_1 \sinh \bar{\alpha}}{\bar{\alpha}(\bar{\alpha}^2 - m^2)} - \frac{d_2 \sinh \beta}{\beta(\beta^2 - m^2)} \right]$$

$$- \left[F_5 \left(\frac{1}{m} \sinh m - \frac{2}{m^2} \cosh m + \frac{2}{m^3} \sinh m \right) \right.$$

$$\left[-F_3(m, \bar{\alpha}, \bar{\beta}) + \frac{1}{3m^2} - \frac{d_1 \sinh \bar{\alpha}}{\bar{\alpha}(\bar{\alpha}^2 - m^2)} - \frac{d_2 \sinh \bar{\beta}}{\bar{\beta}(\bar{\beta}^2 - m^2)} \right]$$

$$+ \sum_{i=1}^{2} \left| F_3(m, \bar{\alpha}, \beta) \left(\frac{d_i \sinh a_i}{a_i} \right) - \frac{d_i F_5}{2} \left(\frac{\sinh(a_i + m)}{a_i + m} + \frac{\sinh(a_i - m)}{(a_i - m)} \right) \right|$$

$$- \frac{1}{m^2}\left(\frac{1}{a_i}\sinh a_i - \frac{2}{a_i^2}\cosh a_i + \frac{2}{a_i^3}\sinh a_i\right)$$

$$+ \frac{d_1 d_2}{\overline{\alpha}}\left(\frac{\sinh(\overline{\alpha}+\overline{\beta})}{\overline{\alpha}+\overline{\beta}} + \frac{\sinh(\overline{\alpha}-\overline{\beta})}{\overline{\alpha}-\overline{\beta}}\left(\frac{1}{a_i^2 - m^2}\right)\right)$$

$$+ \left[\frac{d_i^2}{(a_i^2 - m^2)}\left(\frac{1}{4a_i} - \sinh 2a_i + \frac{1}{2}\right)\right] \qquad \ldots (20)$$

and $$F_5 = \frac{1}{F_4(\gamma, m)}\left[2\gamma m F_1(m, \overline{\alpha}, \overline{\beta}) - 2mF_2(m, \overline{\alpha}, \overline{\beta})\cdot\cosh m\right.$$

$$\left. - \{2\gamma F_2(m, \overline{\alpha}, \overline{\beta}) - 2\gamma^2 F_1(m, \overline{\alpha}, \overline{\beta})\}\ \sinh\ m\right].$$

Now comparing the equation (19) with the Fick's law of diffusion, namely

$$J^* = -D^* \frac{\partial c}{\partial z} \qquad \ldots (21)$$

we get the equivalent dispersion coefficient D^* with which the solute dispreses relative to a plane moving with the mean speed of the flow is obtained as follows:

$$D^* = \frac{v_0^2 h^2}{2D} M_1(m, \overline{\alpha}, \overline{\beta}, \gamma). \qquad \ldots (22)$$

3. Results and Discussion

The equations (20) and (22) show that the equivalent dispersion coefficient D^* depends upon the dimensionless parameters : $\overline{m}$ (chemical reaction rate constant), $\overline{\gamma}$ (surface reaction rate parameter), the viscosity coefficients E_1, E_2, E_3 and the parameters $\overline{K}_i$. The coefficients E_1 and E_2 refer to the flexible behaviour of the microstructure, while E_3 characterizes its rigidity i.e. the higher the values of $|E_1|$ and $|E_2|$ would mean more flexible microstructure while higher values of $|E_3|$ means more rigid microstructure. The parameters $\overline{K}_i$ depend upon the concentration of suspended particles and hence for the numerical calculations have been taken as constants.

It may be pointed out here, that for the particular case when $\gamma = 0$ eqn. (17) reduces to the case of Chandra and Agarwal[1], while $m = 0$ refers to the situation when the dispersion does not undergo any irreversible chemical reaction in the fluid, but has surface reaction at the wall.

The effect of various parameters such as chemical reaction rate constant, m', surface reaction rate constant, γ, and the viscosity coefficients E_1, E_2, E_3 on the equivalent dispersion coefficient can be seen through the function M_1, hence this expression has benn numerically calculated for different sets of values of various parameters. The results are presented by choosing the coefficients $\overline{K}_i$'s as $\overline{K}_1 = 1.1$, $\overline{K}_2 = 1.0$, $\overline{K}_3 = 0.9$ and $\overline{K}_4 = 0.6$ and $A_1 = A_2 = 0.25$.

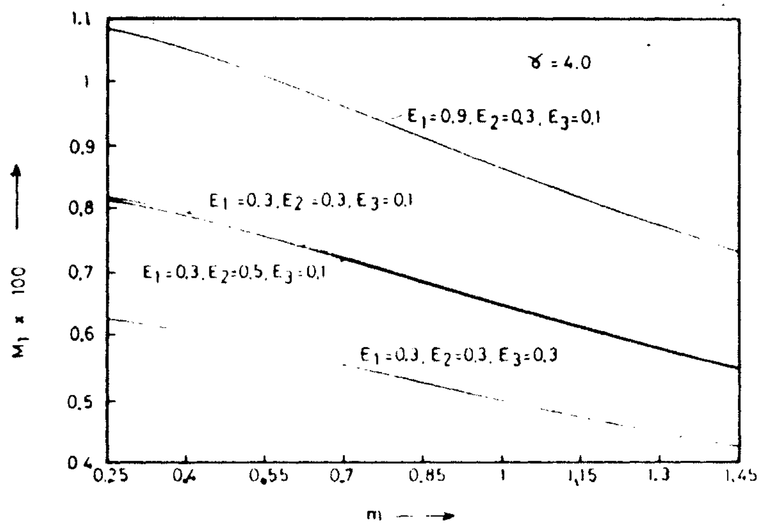

Fig. 2. Variation of M_1 with m for different E_2, E_3.

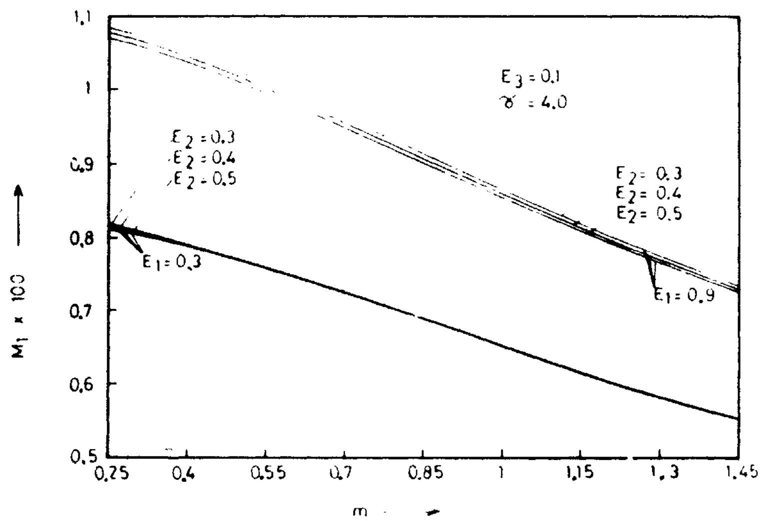

Fig. 3. Variation of M_1 with m for different E_1 and E_2.

The effect of various parameters on M_1 are shown in Figs. 2 to 7. Figures 2-4 show that, for a given simple micro fluid, M_1 decreases as the chemical reaction rate constant 'm' increases. This effect is enhanced as the surface reaction rate constant, γ, increases. The effect of γ on M_1 is further elaborated in Figs. 5 to 7. It is observed from these figures that M_1 shows slight decreases as γ increases from 0 to 2 and then approaches asymptotic value as γ is increased beyond 2. This increase in M_1 with γ, becomes more appreciable as m increases (Fig 7).

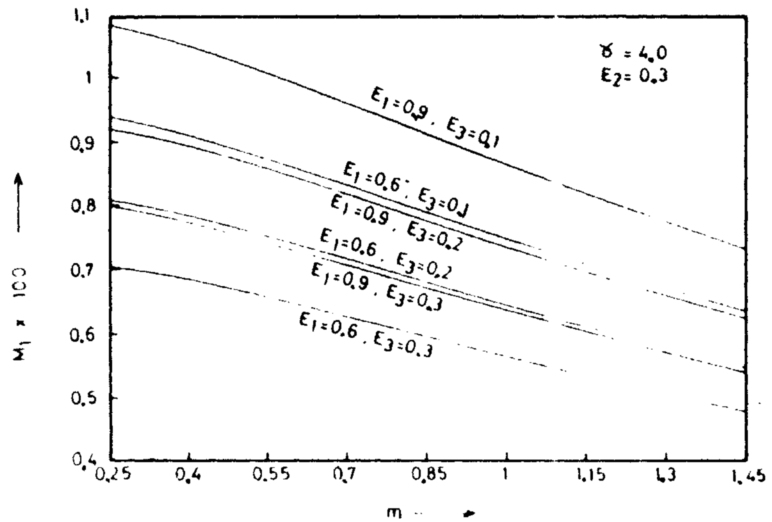

Fig. 4. Variation of M_1 with m for different E_1 and E_3

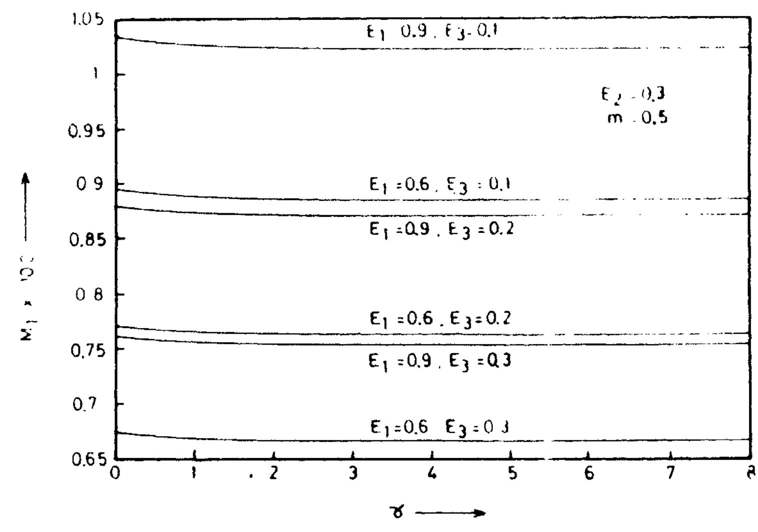

Fig. 5. Variation of M_1 with r for different E_1 and E_3

The effects of simple microfluid parameters in the presence of surface reaction at the wall are depicted in Figs. 2 to 4(with γ = 4.0). These figures show that M_1 increases as the viscosity coefficient E_1 increases, but decreases as the viscosity coefficient E_2 and E_3 increase. However, variation of M_1 with E_2 is not very significant and is almost negligible for smaller values of E_1 (Fig. 3). This behaviour is similar to the case of no surface reaction rate at the wall (γ = 0) Chandra and Agarwal[1]. Combined effects of the viscosity coefficients E_1, E_2, E_3 and γ for m = 0.5 can also be observed through Figs. 5 to 7

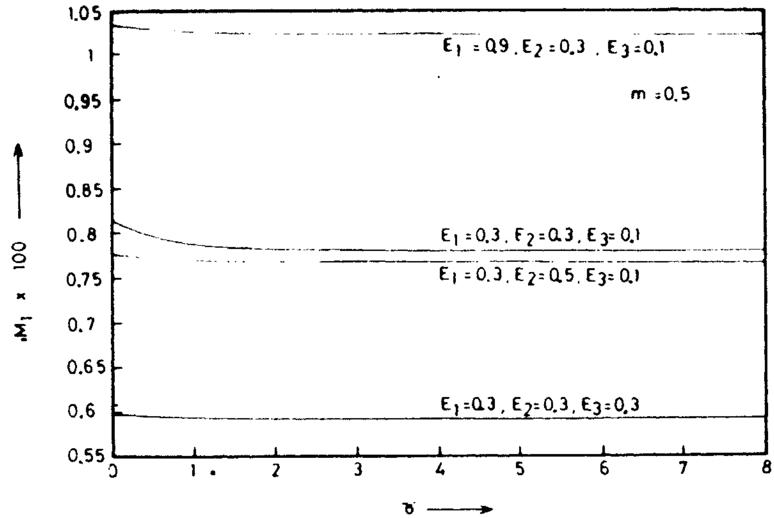

Fig. 6. Variation of M_1 with r for different E_1, E_2 and E_3

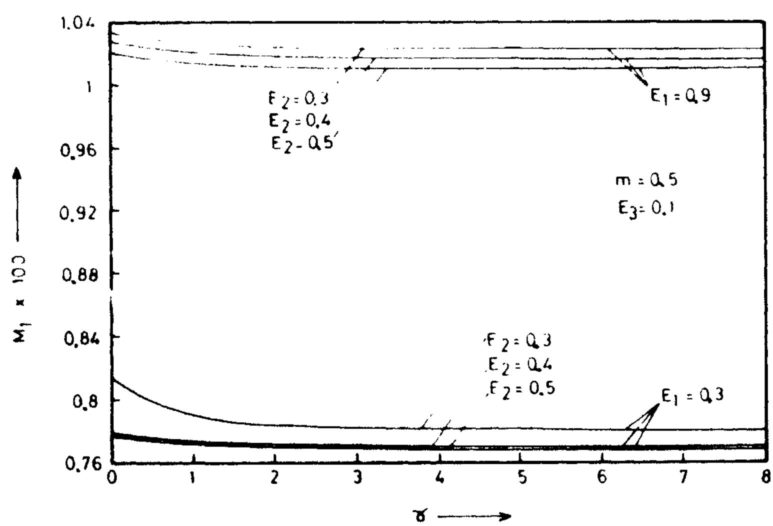

Fig. 7. Variation of M_1 with r for different E_1 and E_2

4. Conclusion

The combined effect of homogeneous and heterogeneous reaction rate constants on D^* is to decrease it for a given set of simple microfluid parameters. The decrease in D^* with homogeneous reaction rate becomes more in the presence of surface reaction on the walls. The equivalent dispersion coefficient decreases as the simple microfluid parameters E_2 and E_3 increases but it increases with the parameter E_1.

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